General Oceanics – KM Contros – ICOS OTC Workshop

7-9 March 2018

Summary: The purpose of this meeting was to discuss experience with, and improvements of, three systems used by stations in the Integrated Carbon Observation System Ocean Thematic Center (ICOS OTC): the General Oceanics underway pCO_2 system, and CONTROS HydroFIA TA and HydroC CO_2 systems. The goal was for participants to come away with a better understanding of the systems and the companies receive feedback and ideas to improve their systems. The meeting should also foster better communication between the vendors and customers. Topics discussed also include: improving atmospheric measurements and synergizing with the atmospheric community, new platforms and new sip recruitment, standardizing data processing and products, and alternative preserving methods for discrete samples.

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G.O.-KM Contros-ICOS OTC Meeting Agenda

When: 7-9 March, 2018
Where: Geophysical Institute, University of Bergen, Norway

Day 1
General Oceanics underway pCO2

9:00 to 9:05: Introductions

9:05 to 9:15: Discuss workshop scope "what participants want out of it," adjust agenda if desired

9:15 to 9:45: Discussion of hardware and documentation (including possible improvements to documentation)

9:45 to 10:30: System and software operation

10:30 to 10:45 Break

10:45 to 12:30: System and software operation (continued)

12:30 to 13:30: Lunch

13:30 to 15:00: Special Topics
Topics Include (but are not limited to)

- Problem Solving/mitigation on G.O. system
- Installing pressure differential sensor between equilibrator and Licor
- Allow various users to demonstrate their (often custom) processing software

15:00 to 15:30: Break

15:30 to 16:30: Ship installation

19:00: Dinner

Day 2
CONTROS HydroFIA TA system and HydroC CO_2 system

Part 1-CONTROS Hydro FIA TA

9:00 to 9:30: Discussion of hardware and documentation (including possible improvements to documentation)

9:30 to 11:00: System and software operation

11:00 to 11:30 Break

11:30 to 12:00 System Demonstration

12:00 to 12:30 Ship installation

12:30 to 13:30: Lunch

Part 2-CONTROS HydroC CO_2 (Underway)

13:30 to 14:00: Discussion of hardware and documentation (including possible improvements in documentation)

14:00 to 15:30: System and software operation

15:30 to 16:00 Break

16:00 to 16:30 System Demonstration

16:30 to 17:00: Ship installation

Day 3
Data Management: Submission, Data Handling, and Coordination

9:00 to 9:30: Submission to the international SOCAT and European *ICOS* networks

9:30 to 10:30: Data reduction and QC procedures
Presentation and Demonstration of QuinCe

10:30 to 11:00 Break

11:00 to 12:00: General discussion on data reduction and QC procedures

12:00 to 13:00: Lunch

13:00 to 13:30 Alternative preserving methods of discrete DIC/Alkalinity samples

13:30 to 14:00: CO_2 in air measurements: Integrating with the Atmospheric Thematic Centre

14:00 to 15:00: Other sensors: Installation and communication between systems

15:00 to 16:00: Discussion of improved coordination, needs, future directions, outreach, and ship recruitment

Minutes Workshop Day 1: *General Oceanics underway pCO2*

*The minutes from the workshop are often paraphrased from the discussion; therefore, they may not perfectly align with the original thoughts of the speaker.

List of Names and Abbreviations

Are Olsen (AO)
Benjamin Pfeil (BP)
Carolina Cantoni (CC)
Charles Roman Battisti (RB)
Denis Pierrot (DP)
Gregor Rehder (GR)
Ingunn Skjelvan (IS)
Kevin Sullivan (KS)
Laurent Coppola (LC)
Maciej Telszewski (MT)
Margot Cronin (MC)
Meike Becker (MB)
Michael Glockzin (MG)
Regis Cook (RC)
Rik Wanninkhof (RW)
Sigve Naustdal (SN)
Siv Lauvset (SL)
Steffen Aβman (SA)
Steve Jones (SJ)
Thanos Gkritzalis (TG)
Tobias Steinhoff (TS)
Tonny Algrøy (TA)
Truls Johannessen (TJ)
Ute Schuster (US)

Discussion of hardware and documentation (including possible improvements to documentation)-No suggestions

Went to Chemistry Lab to discuss the basic principles of the General Oceanics underway pCO2 instrument

Discussion of and suggestions for GO system

Are Olsen (AO): Could you make the software open source, so PIs can make changes to it?

Rik Wanninkhof (RW): Open source could be an issue because it has a lot of flexibility, fail-safes etc. built in to meet the challenge of getting uniform measurements. Therefore, if people can change it, we don't know what effects those changes might be. The 'Black box' design gives a known system.

Kevin Sullivan (KS): Having the ability to interface with different systems could be useful.

Charles Roman Battisti (RB): We would like to be able to send state signals to other systems.

Sigve Naustdal (SN): It would also be useful to be able to configure different running sequences/timings

Tobias Steinhoff (TS): We'd like to be able to integrate the water flow into other systems, and so stop the flow to the GO system as required. Also, to get immediate readouts of values from sensors attached to extra COM ports (e.g. Seabird). We could either do it ourselves or send requests for support of different instrument to GO, but that could be a lot of work for them.

KS: There could be an option to buy the system with open software, but then you don't get support from GO.

AO: Maybe a modular plugin system could be built for the different sensors etc.

RB: Open source would also give opportunity for changes made by the community to be fed back to GO for integration.

SN: Many systems are on research vessels, which share data from several on-board systems via a UDP network. It would be very useful to be able to join this network.

KS: It's on the wish list.

RB: Could we have a visual alarm system so ship engineers can be informed of problems? Maybe yellow/red status lights?

Denis Pierrot (DP): What sort of issues would it signal?

SN: E.g. water flow issues, since that's outside the control of the system.

RW: If you have remote telemetry you'll be able to see it in the data.

RB: But there's still the delay of contacting the relevant person on board.

RW: You'd need to have good criteria of what the signals mean and instructions for how to address them

TS: Water flow is easy to fix on board. A live reading of flow rate would allow the engineers to see it and make adjustments accordingly

SJ: A simple red/yellow probably isn't enough. Having a yellow light mean a number of possible faults still means a lot of work for the engineers to check all the possibilities.

RB/SN: The signal criteria could be customised by the PI

KS: We could have an auxiliary display of various sensor values, highlighted when things need attention.

SN: Including GPS position?

KS: Yes

…

RB: There's a differential pressure sensor in the equilibrator, and we have to use the Licor pressure sensor as an absolute value. This can cause issues because the equilibrator pressure measurement is very important. Could we have an absolute pressure sensor instead, because the Licor sensor isn't as good as we'd like?

RW: I strongly endorse this idea. The increase in expense should be minimal.

SN: We also have to assume that the Licor is at ambient pressure, but there are fans in the box.

KS: The pressure sensor is linked to a vent outside the box

SN/MB: <Describe experiments with additional pressure sensor. See also later presentation>

GR: What's the difference between equilibrator pressure and ambient, and what's the source?

KS: They should be very close, but flow dynamics and water movement caused by the ship have an effect

RB: Also the fact that gas is being removed from the head space

KS: Can be up to 1 mbar

<Brief discussion of ways to measure this – e.g. pressure/flow sensors on the drain>

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TS: It would be good to have a central place for ideas/fixes etc

SL: Been tried several times

RW: Why doesn't it work?

AO: People don't check them for new questions, to add comments etc.

RW: We need to keep trying different approaches because otherwise these workshops are the only places to have these discussions

Ingunn Skjelvan (IS): ICOS has plans to gather this kind of information

RB: If experts aren't looking regularly, then questions won't get answered. So people stop asking. But it's a time sink.

Regis Cook (RC): GO should do a better job with this – we spend a lot of time answering questions, so we could collate that information.

RW: We should decide on this as part of the workshop. GO is an option, but it should be more of a community activity with input from GO. Try to build something that will work, and identify people willing to provide answers. We need several to reduce the workload. Plus it should be widely advertised through by GO, IOCCP etc.

RB: Could it be run as part of the GOOS network infrastructure?

TS: OTC could make a good start on it

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RB: Easier physical access to certain parts of the machine for maintenance would be good, such as better access to the Peltier cooler for replacement.

TS: Also an extension so the wet and dry boxes can be further apart

KS: Purchasing an additional connector would make this possible. <Discussion of how to do it>

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GR: We want to use a Picarro CRDS sensor. What's needed to integrate it? If we want to measure additional gases from a separate stream, how do we manage the flows?

RC: Would need to duplicate all the flow control components

RB: Could you develop two dry box designs? One for Licor and one for Picarro?

MB: Picarro has different control hardware and output specs, so would need a lot of work to integrate it.

RW: It would be good to have different dry box and software versions, and the ability to measure multiple gases/isotopes would be very appealing. The design and requirements should come from the community as per the original pCO2 system.

RC: The second dry box (CRDS) design would need to be community driven

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RW: Request for community input: How often do different components fail? Will help with preventative maintenance, rather than reactive which is what people tend to do currently.

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General Oceanics Uncertainty Analysis

*Presentation by Charles Roman Battisti analysing the uncertainty of the General Oceanics underway pCO2 instrument.

RW: A general question: We use very accurate temperature measurements, and we know the accuracy of the sensors. But how do we know that we're measuring the true equilibrator temperature? It depends on the equilibrator design, the position of the sensor etc.)

KS: [For ICOS requirements] are you going to insist on 2uatm/0.03%? The criteria should be set at a level that is operationally reasonable. For very high coastal values 2uatm probably isn't achievable.

GR: We are also working on the assumption that we are reaching full equilibration. We see differences between them, and this needs looking at in more detail.

RB: Agreed

RW: Note that the 2 μatm is based on the analysis of what's required to constrain the global air-sea flux to 0.1Pg C/yr. The percentage limit is not useful for that.

KS: But that isn't achievable at the coast.

RW: True, but we should specify a larger uncertainty on the coastal ocean fluxes. Relaxing the limits won't help us to improve our estimates.

RB Asked for ideas for further analyses he could do. No suggestions.

GO system special topics

GR: what do we mean with an accuracy of 2 μatm for the fCO2 measurements? This is dependent on the equilibrator type and its response time, and an assessment of its uncertainty needs to be performed. E.g. methane response time is system dependent, and $\tau(CH_4)/\tau(CO_2)$ is somewhere between 25 and 3 (Webb et al 2016). Knowing the equilibrator performance is particularly important when operating in frontal systems, they have seen difference of approximately 8 ppm by using different equilibrators in the same water.

RW: it is important to use equilibrators with fast response time. Alternatively, one needs to know the response time of the equilibrator and do back calculations, but this is not easy. It is of high importance to determine the characteristics of the system, e.g. what is the lag between inlet and equilibrator, how long is the equilibration time etc.

AO: a protocol /cookbook should be made on how to characterize the system, time lag, time constant, etc.

MB gave a presentation on a new absolute pressure sensor, which was installed close to the equilibrator in the wet box at Nuka Arctica. The sensor has high precision and measures the absolute pressure, and the difference between this pressure and the LICOR pressure sensor showed to be approximately 0.8 mbar, which was possible due to a poorly calibrated LICOR pressure sensor.

A question was raised on how often the LICOR pressure sensor needs to be recalibrated. This is not very critical since the system is calibrated using standard gasses.

An important note was made regarding the LICOR6262: 2018 is the last year that LICOR will do maintenance of the LICOR6262. Question if OTC can get hold of as many spare parts for the LICOR6262 as possible from the company before LICOR stops service of them?

RW: the community should check how much the LICORs drift between times of calibrations (comparing calibration sheets before and after the re-calibration).

RW and others answered the question about why LICOR6262 is regarded to be better than the 7000. This is because the 6262 is handling vibrations better than the 7000 (connected to the filament within the sensor/gravity/vibration/swell), and also because the 6262 corrects for both band broadening and water vapor while the 7000 only takes care of the band broadening. Note that the issue with the moving (vibrating) filament has been improved. A suggestion was put forward that OTC could address LICOR and ask for the issue with the filament.

RW: the LICOR840 has a lower cost than the LICOR6262/7000. It is a single beam IR detector, has a water vapor channel, and it might be a good alternative to the 7000. It is being tested now, and it is much noisier than 6262, this is possibly white noise that can be filtered out. The LICOR840 works well on the bench, it is easy to maintain in the field, and it can stand higher temperature than the 6262. More tests are needed.

DP: there is a "wait" function in the GO system. After a period of gas flow the Valco valve close, and the system waits for 10 sec to equalize the pressure (de-pressurize), before a measurements is taken.

RC: before an instrument is sent out it is thoroughly checked; e.g. if the pumps are working properly, several data checks are performed, and equilibrator is checked in water with varying pCO2. The latter shows a reproducibility of 1-2 ppm.

Data transmission via Iridium is occasionally a problem, possibly due to the antenna. The old system (the Neill system), which was originally made for buoys, worked better when it comes to data transmission. Dennis Pierrot et al have a special solution for the deck box, and a publication about this will be available soon.

Air measurements

SL: air measurements are performed on many of the VOS lines, however, how many actually used these data? Currently, atmospheric xCO2 measurements are a core parameter for the marine VOS lines and the required accuracy is 1 ppm (within ATC, the required precision is 0.1 ppm).

GR argued that the atmospheric measurements from VOS lines was of no use.

RW replied that when both sea and air CO2 measurements are performed, the precision is a challenge, but atmospheric measurement from ships are very useful for e.g. calculating fluxes along shore and over sea, for constraining the marine boundary layer, for inverse modelling, validation of atmospheric models, and validation of satellite sensors. Not all calculations needs the high precision as the atmospheric community require. The marine community should aim

for a precision for the marine atmospheric measurements of 0.2 ppm. Currently, an ordinary measurement sequence for a GO system includes 4-5 atmospheric measurements in a row, and if these have a standard deviation (precision) of 0.1 ppm or so, the value is very good.

Test should be made where atmospheric measurements from a GO system are compared with atmospheric measurements using other more precise instruments (e.g. Picarro). **RW and colleagues** have started such a comparison and he encourages ICOS to do the same.

GR pointed out that this is one of the aims for the EU project RINGO (ICOS initiated); comparison between atmospheric (ATC) samples and atmospheric samples from marine instruments (GO system and others).

SL commented that SOCAT will implement routines for checking atmospheric data, as these data are sent in but not yet checked.

Installation on ships

SN presented examples of problems met when a GO system was installed on the cargo ship Trans Carrier; e.g. ship schedule, leakages in seawater pump and tubing, too low flow through the wetbox caused by the flow regulator not opening properly (resolved by removing the flow regulator), impeller house of the seawater pump was too small and the pump did not function properly (resolved by replacing the pump), the Valco valve in the drybox had internal problems with the TX line (resolved by adjusting LabVIEW program) and flooding drain tank (possible due to malfunctioning floats). A very helpful crew solved several of the problems.

Seawater pumps were discussed and it was commented that peristaltic pump should never be used for feeding the pCO2 system with water, because the tubing for these pumps are not CO2 gas tight. Flexible tubing should be minimized because it can adsorb and desorb dissolved gases. It is also advisable to insulate the tubing/pipe supplying the instrument with seawater; particularly the part between the bypass and the system, because the flow is relatively low in this part of the tubing/pipe.

RW: for the future, when biological measurements are to be combined with the CO2 measurements, pumps without impellers should be used, to avoid disturbance of the biological material. De-bubbler has been used by Rik Wanninkhof (RW), and there is no change in pCO2 or O2, however, he prefer not to use it.

RW: Dennis Pierrot et al. will soon publish a paper on ship installation of a GO instrument.

Workshop Day 2: *CONTROS HydroFIA TA system and CONTROS HydroC CO_2 system*

CONTROS HydroFIA TA

Discussion about chemicals

It is possible to refill the chemicals cartridge yourself, but then the accuracy can no longer be guaranteed by KM Contros. KM Contros highlights that there is little experience with refilling

the bags in the cartridge and they need cleaning. Better then to use your own, possibly bigger, bags/containers. That would require fitting a custom extra inlet. This is not prohibitively expensive if done in conjunction with normal maintenance.

Using purified dye is highly recommended by KM Contros.

Frequency of samples. Can be taken at min. 10 min intervals, but how long can the intervals be? The system is closed, so evaporation and salt crystals should not be a problem.

Q: Can the range be changed?

Steffan Aβman (SA): Optimal is +- 200 µmol/kg of the intended middle value, but higher is possible with a loss in accuracy.

Q: How high can the values be? For example, Italy has 2600 µeq/kg average.

SA: KM Contros can calibrate to your working range.

Q: When is the salinity value sent to the system? Timing is important to match the TA measurement.

SA: Often updates of salinity is recommended. The system uses the latest salinity value it got when it measures TA.

Q: Does the cartridge wear out, or can they be used indefinitely?

SA: They do wear, but KM Contros does not know how many times they can be refilled, nor has anyone tried to refill them.

Q: Do the chemicals need heating or cooling if it is placed outside the instrument?

SA: Usually, no. It can freeze, but that seems like the only problem. High temperatures (>40 °C) might cause degeneration of the chemicals as well.

Q: What is a good price for a set of cartridges? EUR100?

Extra inlets can be made for external for "external cartridges".

KM Contros/**Katharina Seelman** will look into taping flexible canisters with gas proof tape.

RW: the dye is not stable at temperatures >40C. This can be an issue for transport and on cargo ships.

RW: the risk of poor data decrease with well prepared chemicals and that it is worth the price. Especially since we are aiming for highly precise and highly accurate data.

Work is done to assess the effect on AT of using impure dye. It is known to have a significant effect on pH, but is less well quantified for AT.

SA: KM Contros use and supply dye with very little impurities for the instruments. It has not been purified.

RW: it is in the community interest to use only one source of dye since this will limit the risk of biases between instruments.

<u>Discussion about drift</u>

There was a discussion about drift and causes of it. Steffen Aβman (SA) claims that drift in early versions were due to issues with the degasser (leaking), creating extra dead space. Drift in newer versions has unknown source, but is fairly linear. The newest version of the system

will have an inlet for a sub-standard, so the system can measure its own drift. Gregor Rehder (GR) points out the possibility of drift being related to stability of chemicals.

One particular user has had problems with their first measurements in port drifting, and need to be excluded. This might be a problem with the particular system, as it has shown suspicious behavior. It might also be explained by fresh water.

Discussion about calibration

It is recommended to calibrate pre- and post-deployment (also in rough environments) and at least once a year. Should also always calibrate after changing/refilling chemicals by the operator using the implemented calibration routine.

There were questions about calibrations while on ships (running continuously). Steffen Aβman (SA) thinks regular sub-standard measurements is sufficient. This now needs to be done manually. Regular sub-standard measurements can be done automatically in the new version of the system, which will have a sub-standard inlet (can be installed on older versions). There is no method to get rid of waste water appropriately if CRMs are used. The mercury chloride does not adversely affect the instrument though.

The waste water of the KM Contros instrument is supposedly non-toxic (as long as no mercuric chloride is used), however, the wastewater is colored blue from the dye. Some people have trouble removing the waste overboard because of the color, despite the waste being non-toxic.

Q: How strongly do you recommend using KM Contros provided cartridge sets? -Left unanswered. There is no study of measurement quality due to impurities.

Discussion about external sensors

The instrument needs salinity, but needs to get it from an external sensor. This is possible to do with serial commands. It may be possible to add UDP as an option in the future. Salinity values can also be changed in post-processing of the data.

Since the measurement is not very sensitive to salinity the system can be set up to read the salinity from the external sensor at the time it closes the sample loop (assuming the external sensor measures frequently enough)

Ship Installation

Recommended flow rate through the pre-filter is 5-20 L/min (preferably towards the lower side to minimize waste water). The instrument needs 50 mL to rinse and measure a sample (~2 mL).

There are no problems with vibrations, but shocks can damage the system.

Maintenance once a year is recommended by KM Contros

Any issues affecting the data are immediately seen since the AT is such a sensitive measurement.

System is Peltier cooled, and insulated, so it should work in both hot and cold condition. In hot, moist conditions moist can be a problem. Use silica-gel inside the housing.

The filter units wears based on use (and if you change flow direction). Claims that is should not need replacement (at least not often).

Upcoming possibilities might include UDP.

RB: which parts are most likely to wear out and this used to be the degasser?

SA: Now it is the CO2-stripper which needs replacement of the CO2 absorbing material after one year run time, and the pump which needs replacement after 6 months run time.

RB: Is there a check list available for engineers to go through to "validate" the system. –Not currently

KM Contros is urged to write a checklist.

SA: A quick start guide is already available for techs.

RB: Will there be a problem if the chemicals run out before the cartridges are replaced?

SA: There should not be. Running the system without water is a problem (due to temperature controls).

AO: can KM Contros implement a shut-down procedure (with standard runs before complete shut down)? -This is apparently hard to automate.

Intercomparison discussion

Laurent Coppola (LC) presents on the results of the FixO3 intercomparison results.

LC: Is ICOS planning to do regular intercomparison/intercalibration exercises (similar to the one done in FixO3)?

Truls Johannessen (TJ): One is planned for 2019

RB: There is still an active decision about where to hold it. Whether it should be at sea or on land. The benefit of it being on land (at a fjord site) is that more people can join and more sensors can join.

Maciej Telszewski (MT): Are there globally implementable recommendations from the FixO3 exercise? Exercises are often very expensive and often not properly followed up by recommendations. Too often results are not published.

LC: The only recommendation to come out of the FixO3 exercise is regarding biofouling

MT: There is a strong need to improve the follow-up and publication of results from intercomparison/intercalibration exercises. IOCCP would be interested in supporting a new exercise, but need a set of defined outcomes first. This is crucial for securing support and funding.

TJ: ICOS is obligated to do intercomparisons/intercalibrations more rigorously and traceable so that we get a better end-product

RW: Companies seem a bit saturated and not too interested in new intercomparisons/intercalibrations. We need to be very clear about the outcomes both for us (scientists, users) and the companies involved.

SA: It is important that the sensors used in intercomparisons/intercalibrations are properly prepared for the exercise and companies need to be directly involved. Objectivity and professionalism is important.

MT: A counterarguement to that is that we need to ensure that the numbers coming out are useful. That may be easier without direct involvement by companies in exercises. We also need to assess, independently, whether the plug-and-play approach works as advertised

SA: Always very important to follow the recommendations about proper use from companies.

GR: Everybody can deploy a sensor and try it, but it is never easy to know what they get out of it. It should not be necessary to involve companies to get intercomparisons/intercalibrations to work properly. That signifies that sensors are not as easy to use as advertised.

Thanos Gkritzalis (TG): GO system follows SOP. IOCCP tried to instigate SOP for sensors. This is not yet done but it is essential to have SOP documents for sensors. The system needs to be binary: either you follow SOP or you do not.

RW: Properly defined operating procedures are key. Remember that SOP are not always followed even when people say they are. The take home message is that if you don't follow SOP then you are out of spec and your data are not as accurate as you may think.

RW: ICOS should implement SOP for sensors (set the rules so to speak)

RB: should the intercomparisons/intercalibrations be attended by the pros from the companies or by the users/scientists that have bought the instruments?

Everyone agrees both, but that scientists are the most important. The user is a key aspect of the total uncertainty.

MT: Since we don't yet have SOP we will need input from both sides. So both companies and users should be involved next year in the ICOS intercomparison/intercalibration

RW: The intercomparison/intercalibration should be used as an opportunity to write SOP

TS: Would be good to have a pre-procedure so that instruments used in the intercomparison/intercalibration next year already have some SOP

RB: There are time issues as well as scale issues (how many sensors to cover, what the facilities can accommodate, cost, etc)

TJ: Planning needs to start immediately

MT: Important to use experience and expertise from the FixO3 exercise

GR: NIVA has a TNA application in to Jerico-Next to do a small intercomparison/intercalibration in November 2018.

RW: what are ICOS requirements? In terms of a reference network the fewer sensors/instruments used the better. It would be smart of ICOS to predefine which sensors are likely to be able to compete with our accuracy requirements rather than invite all

RW: How much of the planned exercise is instrument to instrument comparison and how much is intercalibration of a series of the same instruments?

RW: If SOP are not followed all bets are off and for a network, there needs to be SOPs

RB: the user manuals are the beginning of SOP

RW: ICOS requirements are beginning of SOP also

SA: It would be good to know what the ICOS requirements are and develop SOP from that, then develop sensors based on SOP

[Side note **(SL)**: At a meeting I was at last year someone talked about an intercalibration workshop they had arranged. There they did invite companies and sensor developers but excluded them from parts of the workshop. The companies were not happy about this, but the users liked it because it gave them more freedom to be very honest about their experiences. Maybe that is an approach to try.]

Discussion on recruitment of new platforms and new ships

MT: Does ICOS have a strategy for including new platforms?

TJ: There is a new technologies strategy but this has been postponed because of the labor-intensive station labelling process. Currently there are negotiations with UK, which was supposed to lead that task. Currently, it seems more likely to include new technologies on fixed stations. There are plans for ship liaison also.

MT: Wave gliders are becoming very popular and people are putting all sorts of instruments on them. But there are some data issues. Someone needs to drive the community and take charge of the data to find out the quality of it

RW: PMEL has experience with both wave gliders and sail drones. They have put modified MapCO2-instruments on them with decent success. A limitation of the wave glider is that it has problems with fronts and fast-moving currents

RW: An issue is that VOS lines have water intake at varying depth (down to 11m) but there could be strong gradients near the surface so that pCO2 is actually different on the surface compared to at the intake depth. That makes comparisons difficult. Note that all instruments PMEL have put on sail drones and wave gliders are IR-based.

RW: PMEL also use ISFET pH sensors. Important to recognize the move in parts of the community towards measuring pH and calculating AT from temperature and salinity. Results of that are promising but still a lot of unknowns. Sensor developers tend to be very lucky and get very good data. Then other users struggle much more.

TS: We want to think about the next step in technology and developments that take us there, but many intercomparisons/intercalibrations show that the current sensors are not good enough (ref. the uncalibrated KM Contros sensor being off by 100ppm in the FixO3 study, yet being the best, see **LC** presentation). Many sensors don't work as well as we initially think which is an important consideration for implementing new sensors/new technology on existing platforms.

Discussion moves to contact with shipping lines

TG: It is not easy to add new stations to the ICOS network. Lots of bureaucracy. Would it be possible to move one (existing) station from one platform to another? [Siv: This was not answered by anyone.]

RW: We have had success with cargo ships. There is a big issue about how to approach them. A high level of professionalism is necessary. It can be problem to get ships for desired lines/areas. It is a recurring problem that ships don't stay on the same line forever. Sometimes a ship moves to another part of the world after installation of a pCO2 instrument. An advantage of a global reference network would be that there are people in those other parts of the world that could take over responsibility. Ideally, we also want a ship which has other observations/sensors onboard.

MB: When approaching ships and/or companies it is important to not waste their time. Be well prepared. Know what you need and don't need.

RW: Also need to remember that there are many entities when approaching a ship (owners, ship, crew). Because of this, the success rate is much higher with small companies.

RW: We usually send a brief prospectus to potential ships. 2 pages outlining what, where, who, etc. It is important not to expect too much from the crew. This can be shared with the community.

Benjamin Pfeil (BP): We should produce a professional flyer about us, our instruments, what it involves to host an instrument on a ship, what the benefits are, etc. These can then be handed out to potential ships.

GR: There should be an ICOS brochure showing companies that they are part of something bigger

SA: would it help if we could offer companies a green label if they agree to have our instruments onboard?

MB: That only works with companies that sell things to customers (because customers care). The cargo vessels only care about moving the containers as quickly and cheaply as possible. We are at least 10 years away from a world where emissions and climate policy matters to cargo companies

RW: Recruitment of ships should be lifted up to a much higher (international) level.

TJ: It is an ICOS strategy to contact ship owners directly and try to make accommodations for new instruments already at the ship building phase. This is however still a strategy on paper only. It would be best if one organization takes the role of coordinator for communications with shipping.

Ute Schuster (US): Remember that ICOS is only one part of a global initiative. It would be good to use JCOMM-OBS as a global and cross-platform organization. Currently many different communities (hydrography, carbon, CPR, etc) contact ships independently of each other asking permission to put their instruments onboard. This can cause problems with shipping companies and/or ships that get many uncoordinated requests. There should be better coordination of the scientific communities and scientific communication with ships. Preferably through an existing umbrella organization.

MT: JCOMM-OBS has lobbying power which is important. Rik and Maciej are members and can therefore push things, but it takes funding and quite a lot of time. Remember that we have had this discussion on and off for the past 10 years without getting anywhere. We have never got our act together to aim high enough.

RW: At the SOT [Siv: ship observations team] meeting we had the same discussion so this is something many groups are thinking about

TJ: How quickly can people install an instrument if a ship suddenly offered space?

MT: Good point and it is important to our own capabilities

RW: It is up to each group to know which lines and areas they prioritize. It comes down to time and money.

MT: Perhaps the community needs to consider the OSSE approach more seriously. It is not a word usually heard in the carbon research community

TJ: network design is important to consider, it should not just be any ship or any line but one that improves the network. It may be possible to use the general assembly of ICOS-RI to push for funding towards the kind of coordination efforts mentioned previously

Tonny Algrøy (TA): All ships wanting to fish krill in Antarctic waters need a certain instrument installed [Siv: I did not catch which it was. Sorry.] Maybe that is a way to go.

Workshop Day 3: *Data Management: Submission, Data Handling, and Coordination*

QuinCe presentation

Steve Jones (SJ) presents the current version of QuinCe, the data submission/reduction program that will eventually be used by all stations under the ICOS OTC umbrella. The presentation was recorded and will eventually be available on the ICOS OTC website. The following is from the question and answer section of this presentation.

RW: Will all QC flags (automatic and manual) be saved?

SJ: yes

KS: Can you plot multiple parameters on the same plot?

SJ: Right now it is possible to plot every variable in the system against the others. Need to add more variables in the plots (*?? 2 variables vs time, for example?*)

DP: If ignore one STD, then correction of xCO2 is missing one STD. It ignores the standard for drain time, but it is a standard; ignoring it is an issue.

KS: Then take more time to do the drain.

SJ: This is noted.

RW: How do you treat a standard vs the samples?

SJ: Linear interpolation for offset and across all standards. Check with Dennis software see they give the same results

GR: Do we have to do this (add instrument) for all raw formats we import?

SJ: yes, but you should get raw data which should be in the same format.

RB: The goal for near real time (NRT) stations is to send data directly to QuinCe

BP: Only a lot of work the first time you upload a new format

GR: is there a software that merges STDs? What about the mergings that the instrument software does?

SJ: we need to take as comes from instrument. what the instrument generates, that's what we take; Level 1 data (NRT data) is the goal.

Michael Glockzin (MG): can there be two columns for the same parameter?

SJ: no, then need to define two instruments

MG: what is archived? Raw data or data from table?

SJ: everything. Can later do long term reports, studies and diagnostics which can be useful for e.g. manufacturers

Carolina Cantoni (CC): FOS don't use standards. How is pre and post calibration for FOS stations handled?

SJ: This is not added yet. We need to find out how to handle this, which is open for discussion

SN: Are raw data calibrated to minimum values and can we add coefficients?

SJ: yes, coefficients can be added (so can use raw millivolt values).

TJ: When is QuinCe ready?

SJ: VOS in summer (Aug-Sept). FOS afterwards

GR: will there be a link to label level 2 data

SJ: once is operational, if data needs to relabel, send to QC and instantly re-labeled.

Q: Time span?

SJ: Minutes to get to manual QC. Quick.

MG: Do you have to be online?

SJ: Yes, but future plans to make it offline (issues for synchronizing and so; will likely be implemented in a few years).

MG: Is it possible to throw away columns before import?

SJ: those data that are not identified, they are archived, but will be ignored in the further calc. Good to archive for the future (future processing).

BP: We need RAW data instrument to archive, PIs should not manipulate manually.

KS: Is there a questionable flag, or just good and bad?

SJ: there is also a questionable flag (follows SOCAT).

RW: We put an uncertainty to every value. Flag 2 means better than 2 μatm, Flag 3 (questionable) means outside the standard range. For the questionable values we know what is wrong.

SJ: Good idea. Now we have one flag per row, but in the future it would be nice to have one flag per parameter. Then uncertainty for co2 can be estimated based on the flag.

GR: ICOS put data in the database. Good idea to have a safe storage, but will everything be public?

SJ: Raw data is not public (only on request). Level 1 is limited (can see plots, not data). Level 2 data is completely public.

RB: L1 data maps will be visible on the website, but not the actual L1 data

BP: the world of holding back data is over. Currently requirement from funding agencies and movement towards make them public.

GR: What about PI who want to publish first?

BP: we need a change our culture. Funding agencies demands this.

RB: At one of my previous workplaces, they were allowed to keep the data for a year before making it public. This was to allow the PIs time to get started on publications.

MG: If data is wrong, can we correct it?

SJ: Not yet, but should be possible to re-upload. The technical details are not ready. QuinCe is not the archiving system, but you can export and submit to your own data center, ICOS, SOCAT etc.

MG: So QuinCe calculates pCO2 from raw data. Does this mean I cannot calculate pCO2 myself anymore? After e.g. Dickson?

RW: The purpose is to achieve uniform data reduction. Big advantage to have one package for everybody. But needs to be user friendly. Every station should use this.

SJ: We wish to implement a full audit of calculations. Compare with other methods.

BP: We need to run the same script to ensure consistency

MG: Do we run older data through QuinCe?

SJ: no

AO: Can QuinCe store metadata and ensure full traceability? Calibration coefficients, reports, store serial numbers…

SJ: Yes, metadata should be stored alongside. There are international efforts to standardize metadata. If systems are built sensibly, should be able to link us in. QuinCe won't do this. My view is that we should not duplicate this effort in QuinCe.

RW: QuinCe is online. Calcs and output not in the same place? Storage usage? Preservation of data? Download data to ICOS, but doesn't have the metadata attached.

SJ: Important point, we need to deal with this. Carbon portal have some metadata to identify datasets. Put somewhere: this version of Quince did the processing, to be able to track back.

BP: Software is archived. All in the background is archived.

RB: one way is to approach companies: use a text-based document that QuinCe can pull out and extract info from.

MG: now all pCO2. What about other greenhouse gases?

SJ: not implemented and not planned to implement. Quince can have modules plugged in

BP: from next year we address pH.

GR: Methane discussed in meeting OceanOBS. Need a community agreement about solubility coefficients (and others) to use.

ICOS Data Management

Benjamin Pfeil (BP) presents on ICOS data management. The following is from the question and answer section of this presentation.

RW: We get carried away with the webpage applications. Wrong way to go with web. Eg. different web browser. It's not a secure place to save it. inherently insecure. How difficult to hack into QuinCe and adds a bug? If want uniform data, we need more security thatn the web offers.

SJ: do you use online banking?

RW: yes for convenience

SJ: there are 2 responsibilities here: one on us that it works in reasonable # of browsers, another on users to use the right browsers and keep browser updated. Browsers get better and better.

BP: Everything is documented and archived: can recalculate and go back if get hacked. If you depend on s software, you can get problems with OS, and people not updating software. What's the non-online solution? Online we can at least make sure people use the right version.

SJ: QuinCe follows current standards (use HTTS). QuinCe does not archive data (they are in trusted repositories in data centers with procedures in place). If it's hacked, it can be traceable. We spread responsibility out. Time based backups. Everything can be hacked, but since we have traceability and backups, we can prevent those kinds of things.

RW: it's easier to manage centrally, but for some users may not be the solution (internet speed…).

RB: some will still calculate pCO2

SJ: there will be a transition period. As a scientist you need to get comfortable with that change.

BP: everything online, archive automatically, and faster to make it available. Central access points (f.ex Argo network).

MG: people have their own codes for non-pCO2 data, anyway.

MG: Is Quince code available?

SJ: yes, open source.

MatLAB pCO2 reduction script

Dennis Pierrot (DP) presents on his MatLAB pCO2 reduction script. This presentation used MatLAB directly, so no presentation slides are available. The following is from the question and answer section of this presentation.

Q: Can you zoom in on the blue (problematic data)?

DP: yes

TG: do you use linear interpolation between standard gases?

DP: Yes

SJ: are there limits on how much you can interpolate?

DP: No. Responsibility is on the scientist.

Q: Can you manually input the time offset between the measurements of inlet temperature and the equilibrium temperature?

DP: yes, in minutes. The time offset is not exactly the time of travel, it's a fuzzy number when the inlet and equilibrator temperatures best coincide.

Q: Is the calculated time offset for the whole data set?

DP: yes, the whole data set, which it should be.

RW: what if we change flow for some reason half way:

DP: split the dataset, and treat them with different offsets.

Q: what problem if we don't set the offset.

DP: then the delta T will not be the real delta T, which will lead to an incorrect pCO2.

SJ: does the program move SST (intake temperature) to equilibrator temperature time or vice versa?

DP: everything should be moved to sst value. We move sst and then we move only one record, not everything

Q: can the map have topography?

(general laugh)

Q: can the program produce metadata to send to NCEI

DP: online platform to produce xml file (metadata)

TG: does the program produce uncertainties?

DP: not now, but this can change in the future and we can e.g. move towards assigning uncertainty numbers instead of flags?

RW: the community has a real problem with documentation. It's good to have a system for metadata which is forced and easy, and make it easy to produce metadata. It's nice to have uniformity. QuinCe is also good in that sense. The MatLAB program presented is not so good because you flag your data in a subjective way. So we then need to agree on how to flag.

TG: can the program bracket the standard gases so that everything outside ±1 is removed?

DP: can be done manually. I am reluctant to automate things like this because it's easy to make mistakes.

SJ: That's why QuinCe flags points but doesn't automatically "remove" data. We want to force the PI to look at all automatically assigned QC flags.

DS: Does not exclusively need MatLAB, executable files for non-MatLAB users can be produced.

RW: it is data reducer who decides the QC, both in Denis' MatLAB and Steve's QuinCe programs.

SJ: In the metadata, the PI should write which software was used for data reduction.

RW: is there a difference in output now between QuinCe and the MATLAB program?

SJ: yes

DP: traceability in the metadata: this was processed with this program.

<discussion of integrating discrete samples into data>

KS: Force to 20C instead of SST….?

DP: the program has now been expanded to handle 6 standards (vs 4)

Q: Is QuinCe a replacement for the MatLAB script?

DP and SJ: They are parallel systems

RW: what about documentation?

DP: there is a manual included in the package. There is a steep learning curve.

RW: do you know how many use the MATLAB script?

DP: 8-10 people currently. I inform them about updates.

TG: Is the use of this MATLAB software mentioned when data is submitted to SOCAT?

DP: not automatically.

RW: It should be

<Agreement to add specific field in SOCAT metadata to SOCAT (which software, version number, data and time, used for data reduction)>

CO2 in air measurements; integrating with the ATC

Gregor Rehder (GR) presents on the ICOS ATC requirements and the precision of the ICOS OTC atmospheric measurements.

Q: how many standards does the ATC use?

GR: 3-4 calibration + 2 target gases

Q: are the gases stored flat (horizontal)?

GR: yes. On moving platform, this is not an issue.

RW: recommendations or requirements?

GR: some are requirements (continuous measurements-recommendations slide).

SJ: how to get close to ATC standards, if all atm measurements we take right now are rejected? A bit of worse uncertainty is better than no data.

GR: they see themselves as an entity providing data that meets standards, but for the overall task of ATC setting a global observation network, that may be a point of discussion.

TJ: something to discuss within the ICOS RI meeting

RB: To my knowledge, there are no conversion equations from the atmospheric xCO2 measured by the G.O. system. Therefore, the uncertainty is only in the Licor. Maybe it's qualitative more than quantitative difference in standard gasses. Ask ATC whether they think the standard gases are the problem and not the instrument

SJ: ocean atmospheric data are "locked away and forgotten". We should avoid that the data is not used.

RW: The philosophy is good but rigid. ATC is focused on getting best quality data (0.1 uncertainty). A better uncertainty than this doesn't serve a lot of scientific purpose. Requirements based on best possible measurement, and not the scientific questions. We cannot do better than 0.5 (1 if wet). The most accurate we can get is in marine boundary layer.

GR: it will be effort for us; we have to decide whether to make the effort for the atmospheric community, sort out what we can do that can be useful for ATC, that is also not too much for us, e.g. which frequency and precision is useful for them.

RW: we are not just an ocean community but also a global carbon cycle community. We have to decide if it's useful for us.

US: air CO2 measurement are useful for quality control, that's a benefit for us. For 15 years there was no interest in these data, until last year. Now there is interest from the inversion atmospheric community (starting, but getting there). Another benefit is that this can break barriers between ocean, atmosphere, and land; barriers between observational and model. This is one of the ways of do it. We are a global carbon cycle community. If the ATC does not want our measurements we should still measure. If ATC barriers are so high, we still have other users of these data in the global network.

GR: Stronger interaction with atmospheric science. Inverse modelling will be asking both of us. If we can do a flag of the atmospheric data on the data quality. The data should logically be at the ATC; that is where people will first look for them.

TJ: important to teach the atmospheric community to widen up. Improve atmospheric measurements in the ocean, much better predictions (inversion method).

…

Rik Wanninkhoff (RW) presents on some of the atmospheric results from Miami and UK.

Q: what's the flow rate? (for Ute Schuster's air measurements)

US: rate is 100 ml/min. Air CO2: take out first 10 min of 20 min of data. 1 record every minute. Ship contamination data are removed; everything else stays (e.g. land influence), which increases the standard deviation. Then most data are within 1 uatm standard deviation.

KS: not just local contamination, but also land effect; how do we make sure not to remove too much?

RW: make sure we don't lose signal, Consider standard deviation to remove data points, but something else may be needed.

Discussion on Preserving methods of DIC/Alk samples

Charles Roman Battisti (RB) shows initial results of trying Benzalkonium Chloride (BAC) as an alternative to Mercuric Chloride. BAC tends to foam, which causes inconsistent measurements in discrete measurement systems (i.e. VINDTA, SOMMA). BAC affects alkalinity, so only currently being pursued for DIC measurements.

<discussion about the foaming; try a serial dilution to determine useful concentration to test>

MB: use filter (ex. CONTROS HydroFIA TA filter) to produce seawater that doesn't have biota

Margot Cronin (MC): thymol used for their samples

GR: Zinc chloride produces carbonate precipitate. Didn't follow up.

RB: Nickel Chloride

RB: Acidify sample directly without contact with atmosphere

KS: Headspace is an issue with acidified samples. Small loses can be large. Need to ensure all sample is transferred (i.e. some CO2 being lost to dead space).

DP: good for alkalinity

RB: Nuka they take samples and store alkalinity samples in a dark and cool place. The ship has an approximate 3 week travel time.

MB: Measurements taken 2 times/day

RB: Alkalinity and salinity are taken from the in same bottle

… Southern ocean. space problems.

GR: As a favour to the entire community, please tell us what you find out from the BAC experiments. There is a need for that. Communicate in order to not duplicate efforts.

Other sensors

Comment: several sensors on ship. How to control all systems. Ferrybox providers give the computer that manages the sensors they provide.

RB: GO systems. O2, sal, temp is already taken care of by GO systems. Any pH system commonly used?

KS: Not common, but there is the Sami system.

RB: I've seen some examples of DuraFET systems being used on ships, with just the interface interacting with the seawater, however, I wonder how accurate it is when the body isn't at the same temperature as the seawater

KS: Seabird and other system (Seafet and Durafet), one installed by **KS**, other by technicians from Seabird. The system that was installed by technician has better data. 2 CO2 sensors and 1 discrete. Summer season measurement background is below the detection limit.

RB: Durafet for Argo floats and southern ocean…

KS: OK as long as strong enough signal.

Q: Best practices of installation and management? Is someone doing this on a regular basis, can someone make recommendations?

RB: That is part of my job to help station PIs. Engineer on a regular basis can provide support and better recommendations.

…

RB: For alternative trace gases, is there interest in that for the future?

GR: we're doing some. N2O is becoming essential ocean variable, and are supposed to be measured. CH4 may be less important. Methane use the same sensor so such data will increase as well.

RB: these measurements need specialized standard gases. ATC gets its gases from the CalLAB.

GR: CalLab are setup to provide gases to all ATC stations. The quality we need is less than what ATC wants, but higher than what the calibration gases we now use can provide.

RB: Gregor and Tobias measure trace gases. This requires extra gases. It's going to be hard to produce for small groups (easier in bulk).

GR: The range gets off. Can't get high precision. We need really high concentrations for coastal environment. When coastal component gets more important, it's not an additional problem to produce a couple more standards.

RB: Tobias, you are currently working with a ship-board flux instruments. Other stations may be interested. I know it's still being tested, but it's good for community to know this type of system is coming. However the data output is quite high.

TS: 20 herz.

RB: I want to get a discussion going. What instruments are people interested in incorporating? We have KM Contros and General Oceanics here. Is there anything they should incorporate into their data stream (and communicate further to for ex. The G.O. system)?

TS: on top of ICOS infrastructure, to play around with other measurements. It's not near implementation in ICOS.

GR: early phase of ICOS. Potentially the atmosphere community did some homework. What kind of data we want to have and the specs

TS: what precision we need

RB: Companies like KM Contros and G.O. may like to know if we want to add other sensors.

DP: any system that outputs a digital stream should be possible to add on the G.O.

SN: or analog systems if you have access to the wet box

KS: can combine different sensor with same laptop. It works, but then the technicians need to start the systems.

MB: directly connected. This is complex, so it depends

KS: depends of how big footprint you have.